



chain nodes :

18 19 20 21 28 29 30

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 22 23 24 25 26 27

chain bonds :

1-7 6-18 10-13 18-19 18-20 18-21 21-22 25-28 27-29 29-30

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-17 14-15 15-16
16-17 22-23 22-27 23-24 24-25 25-26 26-27

exact/norm bonds :

6-18 13-14 13-17 14-15 15-16 16-17 18-19 18-20 18-21 21-22 27-29 29-30

exact bonds :

1-7 10-13 25-28

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 22-23 22-27 23-24 24-25
25-26 26-27

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS 21:CLASS
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:CLASS 29:CLASS 30:CLASS